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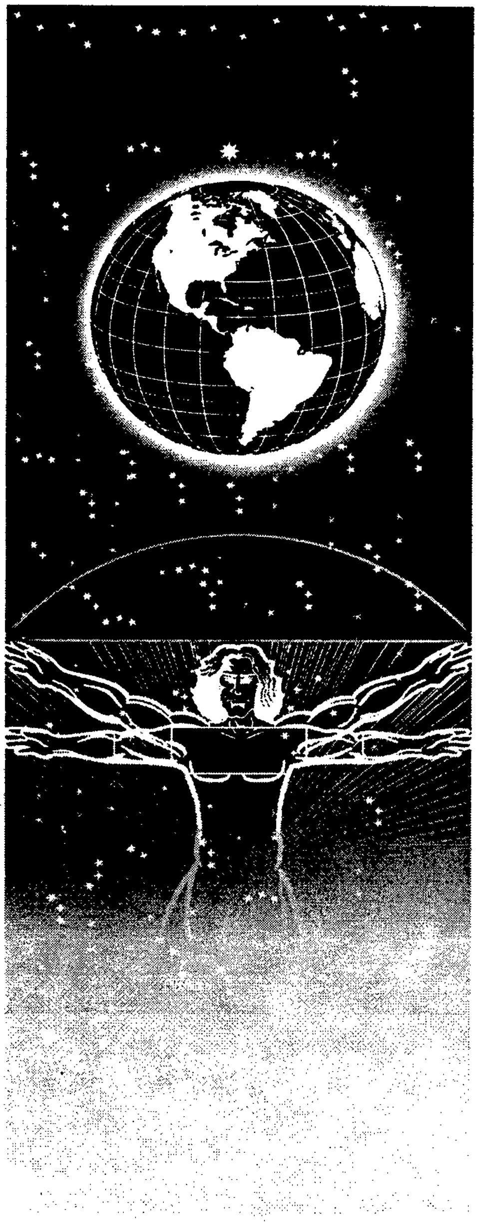

Theoretical Foundations of Growflow

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13. ABSTRACT *(Maximum 200 words)*

A general purpose analysis code has been developed to simulate variably-saturated groundwater flow in a porous media. The code is called GROWFLOW and is based on the SPH analysis method. An improved SPH method called "Gradient SPH" was developed for this effort. Simulation around boundaries and discontinuities is dramatically improved with this new method. Gradient SPH is a Lagrangian method. The governing partial differential equations were cast in a Lagrangian frame of reference for this analysis method. The governing differential equations were then cast into the Gradient SPH formalism. An explicit time integration method is used in the GROWFLOW code, and is therefore conditionally stable. A formulation for calculating the stability limit (largest allowable time step) for the explicit time integration method is presented. GROWFLOW uses a highly flexible method for controlling flow at external boundaries and around internal boundaries. Flow control panels are employed, which are possible due to the Lagrangian nature of the formulation. GROWFLOW has two types of source region models available: constant head and constant velocity. A special treatment for these regions is presented. A method for representing the constitutive relationships with tabular data is presented.

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PREFACE

The work described in this report covers the contract period of July 1995 through April 1996. This work was performed by Applied Research Associates (ARA), Inc., under Contract F08635-93-C-0020, Subtask 8.03, U.S. Air Force AL/EWQ, Barnes Drive, Suite 2, Tyndall Air Force Base, Florida. During the course of this study, there were two project officers, Major Mark H. Smith and Captain Jeff Stinson, BSC. This work was performed under the technical guidance of Mr. Robert E. Walker, ARA. This report was written by Doug Everhart of ARA and edited by Mr. Walker.

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EXECUTIVE SUMMARY

A PC based three dimensional computational procedure has been developed. With this procedure, the engineer will be able to check the design of funnel and gate systems using the site specific properties and conditions.

The name for the PC Smooth Particle Hydrodynamics (SPH) funnel and gate/groundwater flow computer program is GROWFLOW. The code is presently fully operational on a 486 DX2 PC running under the LINUX operating system and has the following capabilities:

1. Fully 3D
2. Handles both saturated and partially saturated flow conditions
3. Saturated hydraulic conductivity can vary throughout the flow domain (can map very complex in situ conditions)
4. Saturated hydraulic conductivity can be orthotopic
5. In-flow conditions can vary with time
6. Handle many sources simultaneously
7. Arbitrarily complex saturation/head and saturation/hydraulic conductivity relationships using look-up tables
8. Features exterior and interior flow control panels to direct and contain flow (build any complex shape desired)
9. No "grid" required (only have to place the integration points so complex shapes are easy to model)

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SECTION I

INTRODUCTION

OBJECTIVE

The overall objective of this program is to develop a three-dimensional analysis tool for the engineer engaged in the design and evaluation of funnel and gate systems.

BACKGROUND

Funnel-and-gate systems are one approach to the remediation of the groundwater which has been contaminated. These funnels (an impervious wall) are used to direct the contaminated groundwater flow into a gate region where remediation can take place. The system serves two basic purposes. First the system directs the flow and thereby contains the contaminant plume and secondly the contaminant in the groundwater is at higher concentrations.

SCOPE

The scope of this study is to develop a PC-based three-dimensional computational procedure for the analysis and design of funnel and gate systems. The approach used is a modified form of Smooth Particle Hydrodynamics (SPH). The resulting computer program is named GROWFLOW.

The GROWFLOW code is extremely flexible. Complex in situ conditions and geometries are easily accommodated. Another important feature of the code is that it can model highly nonlinear systems very efficiently. Convergence is guaranteed. This code operates on a totally different time regime than a typical hydrocode. The stable time step for a hydrocode might be on the order of tens to hundreds of microseconds. The stable time step for GROWFLOW depends on the hydraulic conductivity of the media. The following report summarizes the theoretical base for the procedure.

SECTION II

GROWFLOW SOLUTION ALGORITHMS

In the following sections, the solution algorithms for the GROWFLOW code will be described. First, the explicit time-integration solution method will be discussed, and a flowchart of the time integration loop will be presented. Next, the SPH (Smooth Particle Hydrodynamics) technique that the analysis method is based on will be presented. Then, the partial differential equations (conservation of mass and momentum) will be derived and will be cast into the SPH formalism. Since the explicit time integration method is conditionally stable, a formulation for the propagation speed in the flow field will be presented, along with a derivation of the stability limit for the method. A method for controlling external and internal flow patterns (flow control panels) will be explained. The methods for treating source regions will be described. Finally, the method used for describing the constitutive relationships for the flow media will be presented.

TIME INTEGRATION LOOP

The GROWFLOW analysis code uses an explicit time-integration solution method that will be described in this section. The basis for the time-integration method will be given, and a flowchart of the time integration loop will be presented.

An explicit time-integration solution method was chosen for the GROWFLOW code. There are a few reasons why this is a superior choice for the GROWFLOW code. First, the explicit time-integration method is the method of choice for SPH based techniques. This is necessary because of the nature of the SPH method. Connectivity between integration points is loosely defined, making the assembly of the matrices necessary for implicit time-integration techniques difficult. Next, the behavior of the groundwater flow problem is, in general, highly nonlinear. Because the explicit time integration method uses small time steps, simulation of non-linear effects does not require any additional treatment beyond the normal time-stepping (i.e. subiterations are not required). Finally, the explicit time integration method eliminates the need for the solution of large sets of simultaneous equations. The system of partial differential equations is solved sequentially instead of simultaneously. This can be a big advantage for solving large three-dimensional problems. The memory requirement for the solution is greatly reduced. This allows for solution on a PC class machine, versus a large workstation or supercomputer. Details on the explicit time integration method follow.

The explicit time-integration method is a time-stepping method. Time steps are chosen so that variables change by very small amounts each time step. Variables (functions) are updated at

each time step using the following formula:

$$F^i = F^{i-1} + \left(\frac{dF}{dt}\right)^i \Delta t \tag{1}$$

where,

F^i = Function value at present time step

F^{i-1} = Function value at previous time step

Δt = Time step increment

The selection of a stable time step is critical to the method and will be explained in a later section. For each small time increment, the solution is performed as shown in Figure 1.

SPH SOLUTION ALGORITHM

The GROWFLOW analysis code uses a unique Lagrangian solution technique. The technique is based on SPH techniques. For excellent reviews of the SPH technique and its background see Monaghan, 1992 and Benz, 1989. A discussion of the advantages of the SPH method for groundwater flow simulation will be presented first. A brief description of the original SPH formulation will then be given. The SPH technique that is used in GROWFLOW is completely new and original. A description of this new SPH method, called "Gradient SPH," will be given.

The SPH method has some very important advantages for groundwater flow simulation. Probably the single most important advantage is that it is a fully Lagrangian method. Almost all other groundwater flow analysis codes are Eulerian. The important advantage for Lagrangian codes is that they track material points. This eliminates the expensive "advection" step that Eulerian codes must perform. It also eliminates the "dispersion" effect often seen in Eulerian codes. Sharp, clean material interfaces are preserved.

The SPH method involves the use of arbitrarily arranged integration points that interact with each other through an interpolation function or interpolation kernel. The integration points are dispersed throughout the body to provide a continuum description of the body. The technique is strictly Lagrangian, since integration points represent material points. To aid in the discussion, see Figure 2. Integration point 2 is within the influence zone of integration point 1. Therefore, they can interact. Their interaction is controlled by their separation distance, R, and the smoothing length (typically denoted by h). The value of the interpolation function, W, is a function of R and the smoothing length. There are only two integration points shown in the figure, but an integration point will typically have many different neighbors within its influence zone. Each neighbor within the influence zone contributes to the response of the integration point being considered. By summing up all of the interactions, the behavior of the whole body can be approximated. This can be expressed mathematically with a summation equation:

$$F_i = \Sigma_{j=1}^{N} F_j \frac{m_j}{\rho_j} W \tag{2}$$

where,

F = Any scalar or vector valued function

i,j = Summation indices

N = Total number of integration points that are within influence zone of integration point i

m = Mass

ρ = Density

W = Kernel (interpolation polynomial)

The kernel can have many different forms. Refer to Monaghan, 1992 or Benz, 1989 for a discussion on the rules for choosing and constructing kernels. The kernel that was chosen for the GROWFLOW formulation is an exponential kernel (Benz, 1989). It has the following form for the three-dimensional case:

$$W = \frac{1}{8\pi h^3} exp^{(-v)} \tag{3}$$

where,

h Smoothing length

ν R/h

A completely original form of the SPH technique was developed in this effort. Early versions of GROWFLOW used traditional SPH techniques. Results were not satisfactory in large flow regions, so a new method was developed that would be extremely accurate for any general groundwater flow regime. A new method called "Gradient SPH" was developed for the GROWFLOW code. As the name implies, the method focuses in on the accurate solution of equations involving gradients and differentials. The partial differential equations of motion used to model groundwater flow only involve equations of this type. Consider the set of SPH equations shown above to understand the need for such a formulation.

The need for a gradient-based SPH method can be explained by considering the two SPH Equations (2) and (3). The SPH method is a volume based method. The mass-over-density term in Equation (2) is called the number density function. It is the way weighting is done in SPH. The number density function produces a volume term. Consideration of the kernel function in Equation (3) shows that it produces a one over volume term. This volume weighting procedure works extremely well for areas inside of the body (away from boundaries). Areas near boundaries present a problem. The description of the volume is incomplete, since there are no integration points to sum over outside of the boundary. Groundwater flow problems can be dominated by boundary effects. Clearly a method was needed which is highly accurate in the interior and near the exterior of the solution domain. "Gradient SPH" was developed in response to that need.

The idea behind Gradient SPH is simple, yet powerful. Consider the first derivative of the SPH function in Equation (2) with respect to position:

$$F_i' = \Sigma_{j=1}^{N} \; F_j \; \frac{m_j}{\rho_j} \nabla W \tag{4}$$

Replace the number density function in Equation (4) with the original volume and add a normalization function:

$$F_i' = \zeta_i \; \Sigma_{j=1}^{N} \; F_j \; V_{o_j} \; \nabla W \tag{5}$$

where,

ζ = Normalization function

V_o = Original volume

The normalization function is defined to preserve the gradient, so that the gradient will be accurately reproduced no matter how many neighbors the integration point has (eliminate boundary effects). A normalization function that produces this effect is:

$$\zeta_i = \left[\Sigma_{j=1}^{N} \; V_{o_j} \; (x_i - x_j) \bullet \nabla W\right]^{-1} \tag{6}$$

where,

x = Cartesian coordinates (x = x, y, z)

The set of Equations (5) and (6) are the set of SPH equations that make up the Gradient SPH method. They are the basic SPH equations used in GROWFLOW. An exponential kernel is used in GROWFLOW. The gradient of the kernel function is defined as:

$$\nabla W = \frac{1}{h} \frac{\partial R}{\partial x} \; exp^{\left(-\frac{R}{h}\right)} \tag{7}$$

In order to keep the method symmetric, the smoothing length is defined as:

$$h = \frac{1}{2} \, (h_i + h_j) \tag{8}$$

A nonsymmetric interpolation kernel can be used in GROWFLOW. This is extremely useful in flow fields where the flow is compressing in one direction and expanding in another. In areas where the flow is compressing, greater accuracy can be achieved by allowing the smoothing length to shrink. In areas where the flow is expanding, greater accuracy can be achieved by allowing the smoothing length to increase. This is equivalent to keeping the number zone of influence that is an ellipsoid. The time rate of change of the smoothing length in a particular direction follows the formulation given by Benz, 1989:

$$\frac{dh_x}{dt} = \frac{h_x}{3} \nabla \bullet \vartheta_x \tag{9}$$

where,

ϑ_x = Velocity in a given direction

GOVERNING PARTIAL DIFFERENTIAL EQUATIONS

The governing partial differential equations for groundwater flow in a Lagrangian frame of reference will be derived and will be cast into the SPH formalism in this section. The two partial differential equations of interest are the conservation of mass equation (continuity equation) and the conservation of momentum equation (Darcy's Law). The continuity equation will be derived first and cast into the SPH formalism. The continuity equation will be derived for two different flow conditions: partially saturated and fully saturated. Then the conservation of momentum equation will be presented and cast into the SPH formalism.

The conservation of mass (continuity equation) will be derived and cast into the SPH formalism. Begin by defining some terms that will be used in the derivation:

$$\theta = moisture\ content = \frac{V_w}{V_T}$$

$$\rho = fluid\ density = \frac{m_w}{V_w}$$

$$S = Degree\ of\ Saturation = \frac{\theta}{n}$$

where,

V_w = Volume of fluid

V_T = Total volume (volume of soil plus volume of fluid)

m_w = Mass of fluid

n = Porosity

To proceed with the derivation of the conservation of mass, consider the differential volume shown in Figure 3. The mass of water in this differential element is defined as:

$$m_w = \rho\,\theta\,dx\,dy\,dz \tag{10}$$

Take the derivative of Equation (10) with respect to time to get the time rate of change of the mass of fluid inside of the differential element:

$$\frac{dm_w}{dt} = \frac{\partial(\rho\theta)}{\partial t}\,dx\,dy\,dz \tag{11}$$

The mass flow rate of fluid through the boundary of the differential element in a given direction is defined as:

$$\frac{\partial(\rho\vartheta_x)}{\partial x}\,dx\,A = \frac{\partial(\rho\vartheta_x)}{\partial x}\,dx\,dy\,dz \tag{12}$$

Or, the sum of the mass flow rates through the boundaries of the differential element is:

$$\nabla\bullet(\rho\vartheta_x)\,dx\,dy\,dz \tag{13}$$

The conservation of mass states that the negative of the time rate of change of the fluid mass in the differential element must equal the sum of the fluid mass flow rates through the boundaries of the differential element. Equation (11) must equal Equation (13):

$$-\frac{\partial(\rho\theta)}{\partial t}\,dx\,dy\,dz = \nabla\bullet(\rho\vartheta_x)\,dx\,dy\,dz \tag{14}$$

Simplify Equation (14):

$$-\frac{\partial(\rho\theta)}{\partial t} = \nabla\bullet(\rho\vartheta_x) \tag{15}$$

$$-\frac{\partial(\rho\theta)}{\partial t} = \nabla \bullet (\rho \vartheta_x) \tag{15}$$

Assume that the fluid density does not vary with time or position (the fluid in incompressible). The fluid density term can be moved outside of the derivatives in the right-hand side and left-hand side of Equation (15):

$$-\rho \frac{\partial \theta}{\partial t} = \rho \nabla \bullet \vartheta_x \tag{16}$$

The fluid density can now be eliminated from both sides of Equation (16):

$$-\frac{\partial \theta}{\partial t} = \nabla \bullet \vartheta_x \tag{17}$$

Recall the following identity:

$$\theta = n S \tag{18}$$

Substitution of Equation (18) into Equation (17) yields the final form of the conservation of mass (continuity) equation:

$$-\frac{\partial(n S)}{\partial t} = \nabla \bullet \vartheta_x \tag{19}$$

The conservation of mass equation can be used to calculate the rate at which either the degree of saturation, S, or the porosity, n, changes with time. There are two flow cases to be considered here. For the partially saturated flow condition, the porosity will not change with time. For the fully saturated flow condition, the degree of saturation will not change with time. If these conditions are imposed on Equation (19), the following set of two equations are derived:

$$\frac{\partial S}{\partial t} = -\frac{1}{n} \nabla \bullet \vartheta_x \quad \textit{Partially Saturated} \tag{20}$$

$$\frac{\partial n}{\partial t} = -\frac{1}{S} \nabla \bullet \vartheta_x \quad \textit{Fully Saturated} \tag{21}$$

$$\frac{\partial S}{\partial t} = -\left[\nabla \bullet \left(\frac{1}{n}\, \vartheta_x\right) - \vartheta_x \bullet \left(\nabla\left(\frac{1}{n}\right)\right)\right] \tag{22}$$

Convert Equation (22) to the Gradient SPH form in Equation (5):

$$\frac{\partial S_i}{\partial t} = -\zeta_i\ \Sigma_{j=1}^{N}\ V_{T_j} \left(\frac{\vartheta_{x_j}}{n_j} - \frac{\vartheta_{x_i}}{n_j}\right) \bullet \nabla W \tag{23}$$

Simplify Equation (23) to get the equation used to calculate the rate of change of the degree of saturation for partially saturated flow regions:

$$\frac{\partial S_i}{\partial t} = \zeta_i\ \Sigma_{j=1}^{N}\ \frac{V_{T_j}}{n_j} \left(\vartheta_{x_i} - \vartheta_{x_j}\right) \bullet \nabla W \quad \textit{Partially Saturated} \tag{24}$$

Next, consider the fully saturated condition. Manipulate Equation (21) using the chain rule:

$$\frac{\partial n}{\partial t} = -\left[\nabla \bullet \left(\frac{1}{S}\, \vartheta_x\right) - \vartheta_x \bullet \left(\nabla\left(\frac{1}{S}\right)\right)\right] \tag{25}$$

Convert Equation (25) to the Gradient SPH form in Equation (5):

$$\frac{\partial n_i}{\partial t} = -\zeta_i\ \Sigma_{j=1}^{N}\ V_{T_j} \left(\frac{\vartheta_{x_j}}{S_j} - \frac{\vartheta_{x_i}}{S_j}\right) \bullet \nabla W \tag{26}$$

Simplify Equation (26) to get the equation used to calculate the rate of change of porosity for fully saturated flow regions:

$$\frac{\partial n_i}{\partial t} = \zeta_i \; \Sigma_{j=1}^{N} \frac{V_{T_j}}{S_j} \left(\vartheta_{x_i} - \vartheta_{x_j}\right) \bullet \nabla W \quad \textit{Fully Saturated} \tag{27}$$

Equations (24) and (27) are the conservation of mass (continuity) equations used in the GROWFLOW method. The conservation of momentum equation will be discussed next.

The conservation of momentum equation will be presented and cast into the SPH formalism. The conservation of momentum equation used is a modified form of Darcy's Law, suggested by Huyakorn et al., 1986:

$$\vartheta_x = -k\,K \bullet \nabla(\phi + Z) \tag{28}$$

where,

k = Relative permeability with respect to the water phase (function of S)

K = Saturated hydraulic conductivity tensor

ϕ = Pressure head

Z = Elevation head

The conservation of momentum equation can be cast into the SPH formalism as follows. Rearrange Equation (28) using the chain rule:

$$\vartheta_x = -k\,[\nabla \bullet (\psi K) - \psi \nabla \bullet K] \tag{29}$$

where,

ψ - Total head = ϕ + Z

Convert Equation (29) to the Gradient SPH form in Equation (5):

$$\vartheta_{x_i} = -k_i \; \zeta_i \; \Sigma_{j=1}^{N} \; V_{T_j} \left(K_j \psi_j \; - \; K_j \psi_i\right) \bullet \nabla W \tag{30}$$

Simplify Equation (30) to get the form of the conservation of momentum equation used in the GROWFLOW method:

$$\vartheta_{x_i} = k_i \ \zeta_i \ \Sigma_{j=1}^{N} \ V_{T_j} \left(\psi_i \ - \ \psi_j\right) \ K_j \bullet \nabla W \tag{31}$$

The set of three Equations (24), (27), and (31) form the set of equations that are used to solve the governing partial differential equations in the GROWFLOW method.

PROPAGATION SPEED AND STABLE TIME STEP

A formulation for the propagation speed of a disturbance in a groundwater flow field will be presented in this section. The formulation will be cast into the SPH formalism for use in calculating the stability limit of the solution. The stability limit will be discussed, and the selection criteria for time step size will be given.

The following is a presentation of the formulation for the propagation speed of a disturbance in a groundwater flow field. The partial differential equation is derived in a Lagrangian frame of reference. Start with the governing partial differential equation.

The governing partial differential equation is a modified form of Richard's equation (Therrien, 1992). This equation is obtained by substituting Equation (28), the conservation of momentum equation, into Equation (17), the conservation of mass equation:

$$\frac{\partial \theta}{\partial t} = \nabla \bullet (k \, K \bullet \nabla \psi) \tag{32}$$

Write Equation (32) in indicial notation and split the differential of the total head:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_\alpha}\left(k \ K_{\alpha\beta} \frac{d\psi}{d\theta} \frac{\partial \theta}{\partial x_\beta}\right) \quad \alpha, \beta = x, y, z \tag{33}$$

Make for following definition:

$$D \equiv k \, K \, \frac{d\psi}{d\theta} \tag{34}$$

Substitute Equation (34) into Equation (33):

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x_\alpha}\left(D_{\alpha\beta} \frac{\partial \theta}{\partial x_\beta} \right) \tag{35}$$

Split the partial differential of moisture content with respect to time:

$$\frac{dx_\alpha}{dt} \frac{\partial \theta}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha}\left(D_{\alpha\beta} \frac{\partial \theta}{\partial x_\beta} \right) \tag{36}$$

The speed of propagation in a particular direction is defined as:

$$C \equiv \frac{dx}{dt} \tag{37}$$

Substitute the definition in Equation (37) into Equation (38):

$$C_\alpha \frac{\partial \theta}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha}\left(D_{\alpha\beta} \frac{\partial \theta}{\partial x_\beta} \right) \tag{38}$$

Expand Equation (38) using the chain rule:

$$C_\beta \frac{\partial \theta}{\partial x_\beta} = \frac{\partial D_{\alpha\beta}}{\partial x_\alpha} \frac{\partial \theta}{\partial x_\beta} + D_{\alpha\beta} \frac{\partial^2 \theta}{\partial x_\alpha \, \partial x_\beta} \tag{39}$$

Eliminate the first partial differential of moisture content from Equation (39):

$$C_\beta = \frac{\partial D_{\alpha\beta}}{\partial x_\alpha} + D_{\alpha\beta} \frac{\partial \theta}{\partial x_\alpha} \tag{40}$$

Insert Equation (34) into Equation (40):

$$C_\beta = \frac{\partial}{\partial x_\alpha}\left(k \; K_{\alpha\beta} \frac{d\psi}{d\theta} \right) + k \; K_{\alpha\beta} \frac{d\psi}{d\theta} \frac{\partial \theta}{\partial x_\alpha} \tag{41}$$

Insert Equation (18) into Equation (41), and note that head is not a function of porosity:

$$C_\beta = \frac{\partial}{\partial x_\alpha}\left(\frac{k}{n}\, K_{\alpha\beta}\, \frac{d\psi}{dS}\right) + \frac{k}{n}\, K_{\alpha\beta}\, \frac{d\psi}{dS}\, \frac{\partial (nS)}{\partial x_\alpha} \tag{42}$$

Rewrite Equation (42) in tensor notation:

$$C = \nabla \bullet \left(\frac{k}{n}\, K\, \frac{d\psi}{dS}\right) + \frac{k}{n}\, \frac{d\psi}{dS}\, K \bullet \nabla (nS) \tag{43}$$

Equation (43) is the partial differential equation for speed of propagation. The derivative of head with respect to degree of saturation is a constitutive relationship and will be discussed in a later section. The last step is to cast it into the SPH formalism.

The speed of propagation equation can be cast into the SPH formalism as follows. Rearrange Equation (43) using the chain rule:

$$C = K \bullet \nabla\left(\frac{k}{n}\, \frac{d\psi}{dS}\right) + \frac{k}{n}\, \frac{d\psi}{dS}\, \nabla \bullet K + \nabla \bullet \left(k\, K\, S\, \frac{d\psi}{dS}\right) - nS\, \nabla \bullet \left(\frac{k}{n}\, K\, \frac{d\psi}{dS}\right) \tag{44}$$

Convert Equation (44) to the Gradient SPH form in Equation (5):

$$C_i = \zeta_i\, \Sigma_{j=1}^{N}\, V_{T_j} \left[K_i \frac{k_j}{n_j}\left(\frac{d\psi}{dS}\right)_j + K_j \frac{k_i}{n_i}\left(\frac{d\psi}{dS}\right)_i + k_j K_j S_j \left(\frac{d\psi}{dS}\right)_j - \frac{n_i}{n_j} k_j K_j S_i \left(\frac{d\psi}{dS}\right)_j \right] \bullet \nabla W \tag{45}$$

Equation (45) is the final form of the equation used to calculate speed of propagation. The speed of propagation can be used to calculate the stability limit of the calculation.

The explicit time integration used in GROWFLOW is "conditionally stable". A time step increment must be used that is smaller than the stability limit for the solution. If the time step increment is too big, the solution will become unstable and numerical oscillations will grow very quickly. Fortunately, there are rules for estimating the stability limit for a calculation.

The stability limit can be estimated for a particular solution. The stability limit for an explicit time integration solution is generally the time it takes for a disturbance to travel a "characteristic length". A characteristic length for a finite element solution is the length of the

The stability limit can be estimated for a particular solution. The stability limit for an explicit time integration solution is generally the time it takes for a disturbance to travel a "characteristic length". A characteristic length for a finite-element solution is the length of the side of an element. In SPH solutions, it is the smoothing length, h. No time step increment can be larger than the time it takes a disturbance to travel a smoothing length. This can be stated mathematically:

$$\Delta t \leq \frac{h}{C} \tag{46}$$

The procedure used in the GROWFLOW code is to find the smallest combination of smoothing length over speed of propagation, and then multiply this by a safety factor. The time step increment is calculated using the following equation:

$$\Delta t = \lambda \left(\frac{h}{C}\right)_{min} \tag{47}$$

where,

λ = Factor of safety (0.5 is used in GROWFLOW)

A new time step increment is calculated every time step using Equation (47).

SECTION III

FLOW CONTROL PANELS

Flow control panels will be discussed in this section. Flow control panels are used in GROWFLOW to limit flow at the external boundaries and to create internal boundaries in the solution. The characteristics of the flow control panels, how they operate, and were they may be used will be explained in the following discussion.

Flow control panels have the following characteristics. They are quadrilateral shapes that are described by four corners. They are assumed to have no thickness. Any arbitrary shape can be assembled with the panels (similar to using finite element shell or plate elements to describe a shape). The panels are used to control flow through the area within the limits of the panel edges.

The flow control panels operate by preventing flow normal to the surface of the panel from occurring. They form an impermeable boundary. They can be used on the external boundaries to prevent fluid from flowing out. This is equivalent to putting sides on a tank. They can be used in the interior to prevent flow through an area. Flow parallel to the panel is not restricted.

The algorithm for the panels works in the following way. Fluid is not allowed to penetrate the panel. All of the fluid particles that are within a small capture zone near the panel are checked for penetration at each time step. If the motion of the particle would result in penetration of the panel, the velocity component normal to the panel is set to zero. This prevents penetration while still allowing motion parallel to the panel. Also, the penetration point must be within the boundaries of the edges of the panel.

The flow control panels can be used on the exterior or in the interior of the problem. A separate type of panel is used for each situation. The interior panel differs from the exterior panel in one very important way. Interior panels do not allow interactions to occur between particles on opposite sides of the panel. Exterior panels do not check for this condition and should not be used in the interior of the problem. The need to check for interactions and limit interactions is the result of the nature of SPH. Recall that SPH integration points (particles) interact with all of the neighbors within an influence zone (two times the smoothing length).

This occurs through a summation (integration) process. An interaction between two neighbors separated by a flow control panel must be prevented to model physical reality.

Flow control panels are an excellent tool for modeling the physical impermeable boundaries of a problem. They can also be used to precisely model internal impermeable boundaries such as walls.

SECTION IV

SOURCE MODELS

The two source models available in GROWFLOW will be described in this section. They consist of a constant head source model and a constant velocity source model. The common theory behind, and operation of, the source models will be discussed first, then each model will be described.

A special procedure must be used for the source models in GROWFLOW. This procedure consists of defining the integration points (particles) that make up the source, defining the source panel, and injecting particles from the source into the flow field. Recall that the SPH method is a Lagrangian method. Material points are tracked in the solution. All of the material in the solution must be defined at the beginning of the solution. That means that the material that flows in from the source regions must be accounted for (defined) at the beginning of the solution (see Figure 4). A set of particles are defined as source particles (shown in red). The source particles move through the source region perpendicular to the source panel. The source panel is a quadrilateral defined by four points, just like flow control panels. As the particle approaches the source panel, a check is made to see if the source particle penetrates the source panel. If penetration occurs, injection of the source particle into the flow field occurs. The particle is converted to a normal flow field particle. Particles in the source region can only interact with regular flow field particles through the source panel. This was done to limit interactions to just the area around the source panel. This is of practical importance for modeling interior sources in the flow field.

Note that the source models in GROWFLOW only allow one-way flow. That is, only source particles can pass through the source panel. Regular flow field particles cannot move into the source region. This simply means that the source models should not be used to model sinks. A better way to model sinks in GROWFLOW is to simply provide a volume for fluid to flow into. There are two types of source models in GROWFLOW.

A constant head source model is available in GROWFLOW. Inflow velocity is adjusted so that a constant, predefined head is maintained in the source region.

A constant velocity source model is available in GROWFLOW. The head in the source region is adjusted so that a constant, predefined inflow rate is maintained.

SECTION V

CONSTITUTIVE MODELS

The constitutive models used in GROWFLOW will be described in this section. There are two constitutive relationships that must be defined for a groundwater flow analysis: the relationship between degree of saturation and pressure head, and the relationship between degree of saturation and relative permeability. These two relationships will be discussed, then the method for describing these functions in GROWFLOW will be explained.

There are many different functional relationships that have been used to describe the relationship between degree of saturation, S, and pressure head, n, and the relationship between degree of saturation, S, and relative permeability, k. As Therrien (1992) points out, any physically realistic relationship can be used. A great deal of flexibility can be added to an analysis code by using a tabular method for describing the constitutive relationships. No restrictions are then placed on how complex the relationships can be. A tabular method for describing the constitutive relationships is used in GROWFLOW.

The tabular method used in GROWFLOW consists of representing the constitutive relationship data with a piece-wise linear fit. Figure 5 shows how the piece-wise linear fit is made to the constitutive relationship data. Any desired point on the curve is found by linearly interpolating between two points on the piece-wise linear fit curve.

SECTION VI

SUMMARY AND CONCLUSIONS

A general purpose analysis code has been developed to simulate variably-saturated groundwater flow in a porous media. The code is called GROWFLOW and is based on the SPH analysis method. An improved SPH method called "Gradient SPH" was developed for this effort. Simulation around boundaries and discontinuities is dramatically improved with this new method. Gradient SPH is a Lagrangian method. The governing partial differential equations were cast in a Lagrangian frame of reference for this analysis method. The governing differential equations were then cast into the Gradient SPH formalism. An explicit time integration method is used in the GROWFLOW code, and is therefore conditionally stable. A formulation for calculating the stability limit (largest allowable time step) for the explicit time integration method is presented. GROWFLOW uses a highly flexible method for controlling flow at external boundaries and around internal boundaries. Flow control panels are employed, which are possible due to the Lagrangian nature of the formulation. GROWFLOW has two types of source region models available: constant head and constant velocity. A special treatment for these regions is presented. A method for representing the constitutive relationships with tabular data is presented.

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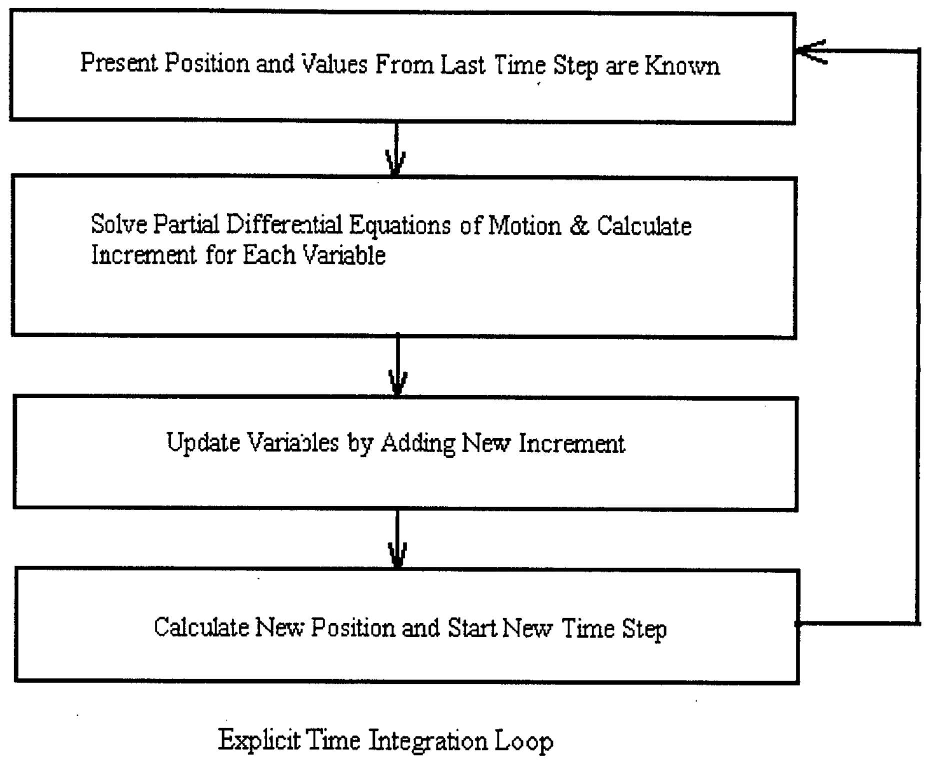

Figure 1. Solution Flow Diagram.

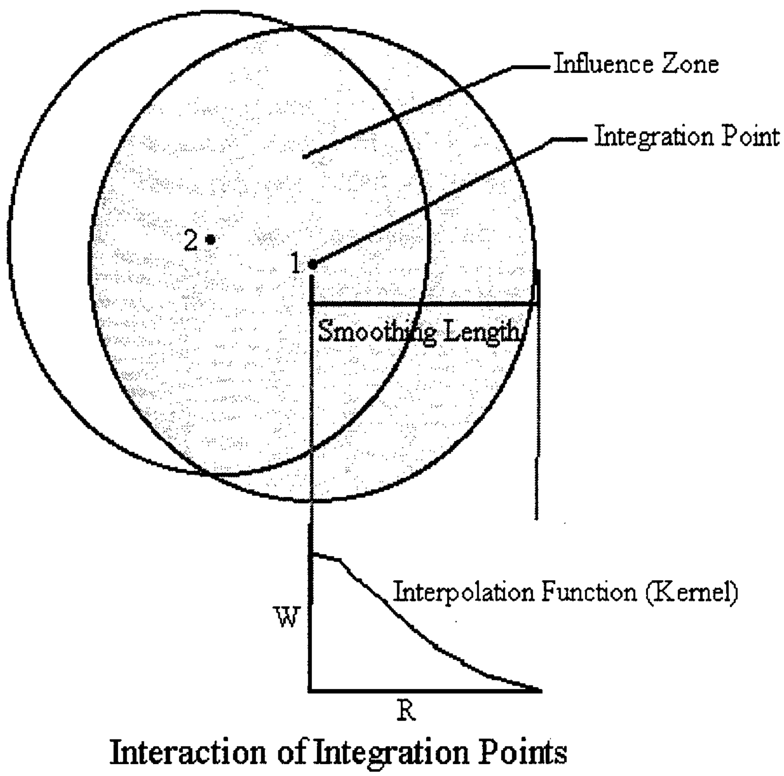

Figure 2. Interaction of Integration Points.

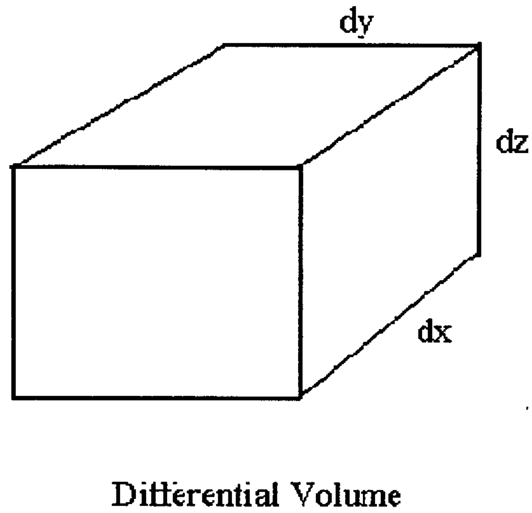

Figure 3. Differential Volume.

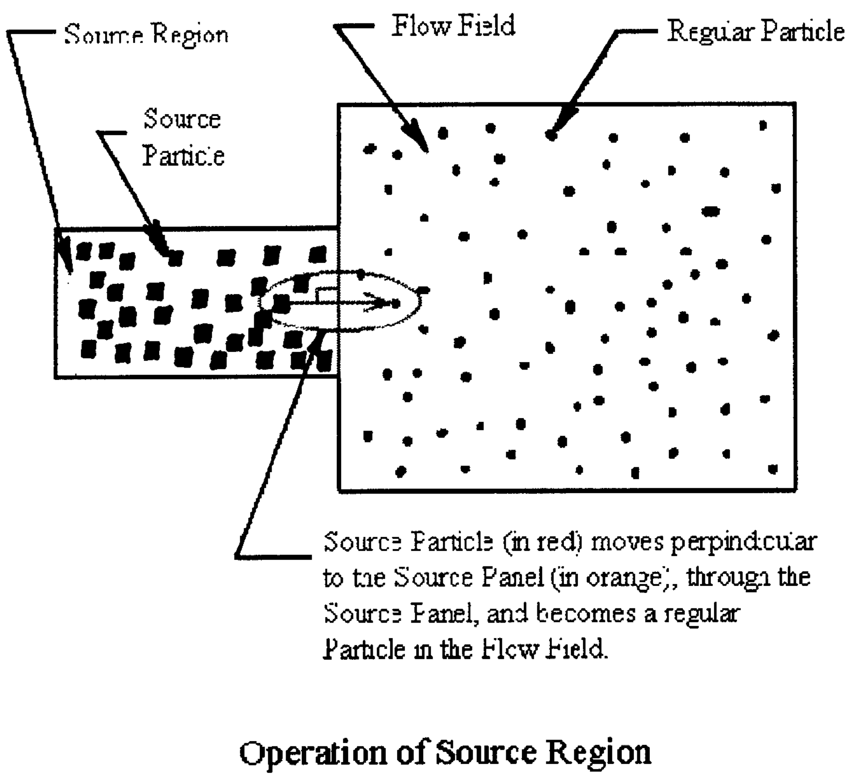

Figure 4. Operation of Source Region.

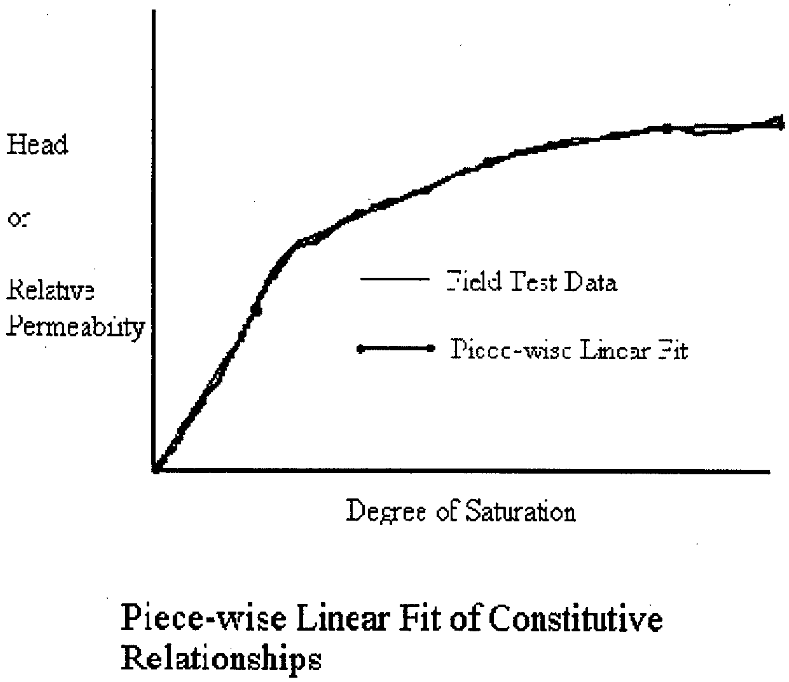

Figure 5. Piece-Wise Linear Fit of Constitutive Relationships.